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Novel Ni-Based Ohmic Contacts To *n*-SiC For High Temperature and High Power Device Applications

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Abstract

Novel Pt/Ti/WSi/Ni composite ohmic contacts to *n*-SiC were investigated as a function of annealing temperatures up to 1000 °C. The onset of ohmic behavior occurred after annealing at 900 °C. Annealing at temperatures between 950 and 1000 °C yielded excellent ohmic behavior. At these temperatures the contact-SiC interface was smooth, defect free and characterized by a narrow Ni_2Si reaction region. The annealed contacts possessed smooth surface morphologies and exhibited minimal contact expansion. The residual carbon, resultant from SiC decomposition, was constrained by reaction with the WSi and Ti metallization layers forming carbide phases of W and Ti. The locations of the carbide phases were spatially distant from the metal semiconductor interface. The anneal optimized (annealed at 950 and 1000 °C for 30 s) Pt/Ti/WSi/Ni ohmic contacts to *n*-SiC were evaluated for thermal stability via pulsed/cyclic thermal fatigue and aging experiments at 650 °C. Negligible changes in the electrical properties, microstructure, and surface morphology/roughness were observed for both annealed ohmic contacts in response to 100 cycles of acute cyclic thermal fatigue. Aging of the 950 °C annealed contact for 75 hours at 650 °C resulted in electrical failure and chemical interdiffusion /reaction between the contact and SiC substrate. The 1000 °C annealed contact retained omicity after 100 h of aging and was found to be chemically and microstructurally stable. These findings indicate that the 1000 °C annealed Pt/Ti/WSi/Ni ohmic contact to *n*-SiC is thermally stable and merits strong potential for utilization in high temperature and pulsed power devices.

I. Introduction

Recently, wide bandgap semiconductors such as SiC have attracted much attention for high power, high temperature, high frequency, and high radiation tolerance device applications. It is the exceptional properties of SiC, such as, high breakdown field, large bandgap, high thermal conductivity and large electron saturation velocity, which are responsible for these device application interests [1, 2]. It has been reported that most SiC based electronic devices, which cannot sustain long-term operation at elevated temperature/power levels, suffered deterioration of their metal/SiC contacts [3]. Thus, an important concern for realization of SiC devices is the formation of low resistance ohmic contacts with good thermal, chemical, and mechanical stability. The development of such ohmic contacts serves to insure enhanced device reliability under the influence of high power and high temperature in-service operational stress.

To date, many metallizations, namely, Ni, Al/Ni/Al, Cr, Al, Au-Ta, TaSi$_2$, W, Ta, Ti, Ti/Au, TiSi$_2$, Co, Hf, and WSi have been investigated for ohmic contacts to n-SiC [2-4]. Ni ohmic contacts have been suggested as superior candidates due to their reproducible low specific contact resistance, less than 5.0 x 10^{-6} ohms-cm^2, and deemed the industry standard ohmic contact to n-SiC [2, 4-6]. Fabrication of Ni ohmic contacts requires a post deposition anneal at temperatures ranging from 950 to 1000 °C. This anneal causes the Ni to react with SiC to form Ni$_2$Si and is responsible for achieving ohmic behavior [4, 6, 7]. However, the annealing process also causes undesirable features, namely, broadening of the metal SiC interface, a rough interface morphology heavily laden with Kirkendall voids, carbon segregation at the metal-SiC interface and/or throughout the metal layer, and substantial roughening of the contact surface [5-8]. Thus, even though Ni contacts possess excellent electrical properties, the above mentioned features will inhibit long term reliability and ultimately cause device failure via contact degradation and/or wire bond failure after exposure to extensive high power and high temperature device operational stresses.

The goal of this investigation was to eliminate the undesirable features (residual carbon, void formation, and rough surface morphology) associated with Ni ohmic contacts by designing, fabricating, and optimizing an improved ohmic contact, to n-SiC for high power and high temperature device applications. Subsequent to contact optimization the contact reliability was evaluated via both static and pulsed thermal stability-reliability testing.

II. Experiment

The Pt/Ti/WSi/Ni (100nm/25nm/80nm/40nm) composite metallization was sputter deposited (WSi) and e-beam evaporated (Ni, Ti, Pt) on research grade (0001) Si-faced 4H n-type (8.0x10^{18} cm^{-3}) SiC wafers. The samples were rapid thermally annealed (RTA) in an AG Associates rapid thermal annealing system for 30 s at 900, 950 and 1000 °C in a N$_2$ atmosphere. Material characterization was performed on the as-deposited and annealed samples. The contacts electrical quality was evaluated via current-voltage (I-V) characteristics using a HP 4140B semiconductor test system. Auger electron spectroscopy (AES) was used to chemically depth profile the different contact elements. The AES data was acquired using a Perkin-Elmer PHI660 scanning Auger microscope. A 5 keV electron beam was used to stimulate Auger transitions within the sample. In addition, a 4 keV Ar$^+$ ion beam was used to simultaneously sputter-etch the surface with a sputter rate of 10Å/s. In this way, elemental information as a function of depth was collected, that is, an Auger depth profile. Field emission scanning electron microscopy (FESEM) was utilized to assess the contact surface morphology, contact-SiC interface uniformity, and film microstructure. The surface morphology was also examined and quantified by a Digital Instrument's Dimension 3000 atomic force microscope (AFM) using tapping mode with amplitude modulation. The contact structure was analyzed by glancing-angle (5°) x-ray diffraction (GAXRD) via a Siemens D-5005 powder diffractometer using Cu K$_\alpha$ radiation at 50 kV and 40 mA.

The anneal optimized contacts (950 and 1000 °C annealed contacts) were subjected to

continuous thermal stress at 650 °C, referred to as static thermal fatigue or aging, for up to 100 hours in a tube furnace with an ambience of nitrogen. An identical set of contact samples were subjected to pulse or cyclic thermal stress. The pulse thermal fatigue tests were conducted in an AG Associates RTA system with an ambience of nitrogen, for 1, 10, 30 and 100 cycles at 650 °C with a pulse width of 10 s followed by a 60 s cool. In order to evaluate the electrical integrity of the contacts as a function of thermal fatigue duration, I-V measurements were acquired after specified intervals (after 1, 10, 40, and 100 cycles for pulsed thermal fatigue testing and after 1, 24, 50, 75, and 100 h for the aging experiments) of fatigue exposure. The contacts structural, compositional, microstructural, interfacial and surface quality were assessed prior and subsequent to thermal fatigue exposure.

III. Results and Discussion

The electrical, structural, and chemical properties of the Pt/Ti/WSi/Ni ohmic contacts to n-SiC were investigated as a function of annealing temperature. The I-V characteristics of the as-deposited and annealed composite contacts to n-SiC are displayed in Fig. 1. The as-deposited sample exhibited rectifying behavior suggestive of a large barrier height, typically 1 eV or greater. Annealing at 900 °C caused the I-V characteristics to move toward ohmic behavior. Ohmic behavior is demonstrated by I-V characteristics which posses linear characteristics with small resistance and are symmetric with reversal of voltage polarity. The contacts became fully ohmic after the 950 °C anneal. A slight reduction in resistance, with respect to the 950 °C annealed contact, was achieved after annealing at 1000 °C. Thus, annealing at temperatures between 900 and 1000 °C significantly enhanced the current conduction through the contacts.
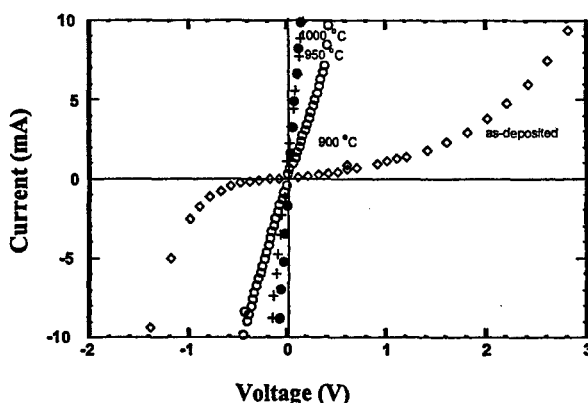

Figure 1: I-V characteristics of the as-deposited (open diamonds), 900 °C (open circles), 950 °C (crosses), and 1000 °C (filled circles) annealed Pt/Ti/WSi/Ni contacts to n-SiC.

In order to assess and understand the contacts electrical characteristics AES elemental depth profiles, GAXRD, and FESEM microstructural analyses were performed on the as-deposited and annealed samples. The AES depth profiles for the as-deposited and 1000 °C annealed samples are displayed in Fig. 2. In the case of the as-deposited Pt/Ti/WSi/Ni composite contact the layer structure between each of the contact metallizations remains

distinct. Figure 2a clearly shows that the top surface is composed of pure Pt. Underlying the Pt is a very well resolved Ti layer. The Ti layer shows signs of oxidation as evidenced by the oxygen signal peaking at ~18 at% at a sputter time of 250 s. The WSi and Ni layers are very distinct and show no evidence of mixing. The interface between Ni and SiC substrate is chemically abrupt; that is, there is no evidence of an interfacial oxide or interfacial chemical reactions upon sputter deposition. The AES depth profile of the 1000 °C annealed sample is shown in Fig. 2b. The individual contact metal layers are no longer distinct. Extensive intermixing has occurred in response to the 1000 °C heat treatment. A minimum of four layers are present within the contact metallization. The top or outer most layer is dominated by Pt, Ni, Si, and W signals and most likely consists of several phases or alloys. Underlying the surface alloy zone is a layer composed predominately of tungsten carbide. Beneath the tungsten-based layer is a region where the carbon signal displays a strong peak, 55 at. %, at a sputter time of 750 s. The position of the carbon peak coincides with the maximum in the Ti signal and is suggestive of TiC phase formation.
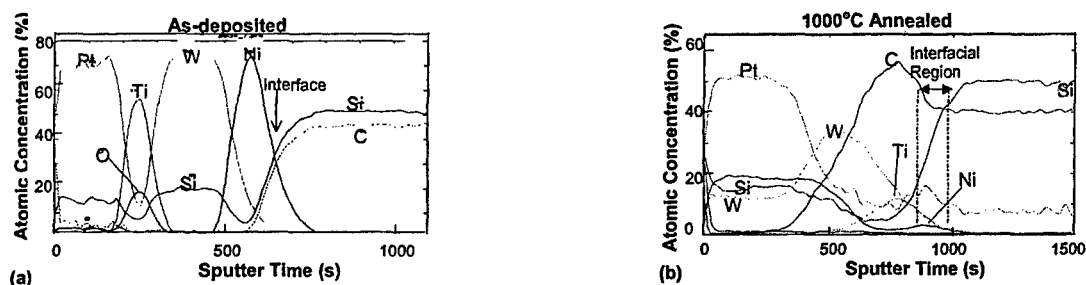

Figure 2: AES depth profile for (a) the as-deposited and (b) the 1000 °C annealed Pt/Ti/WSi/Ni metallization scheme on n-SiC.

The presence of TiC was confirmed by the GAXRD analysis. GAXRD analysis on the 1000 °C annealed sample revealed peaks at 41.7°, 72.35°, and 90.8° two theta which correspond to 2.16 Å, 1.30 Å, and 1.09Å d-spacings for TiC. The 20-80 at. % decay of the Si signal, between 850 s and 950 s sputter time, defines the metal-SiC interfacial region. Within this designated interfacial region exists a peak in the Ni signal. We suggest this to be evidence of a limited reaction region between Si and Ni resulting in Ni_2Si phase formation at the metal-SiC interface. Within this same area is a Pt peak, which has, been attributed to noise at the Pt energy level. The GAXRD data also supports the existence of the Ni_2Si phase at all annealing temperatures. The GAXRD analysis (not shown) detected peaks at 32.78°, 33.4°, 36.6°, 43.9°, 50.9°, and 52.8° two theta which correspond to the d-spacings of 2.73 Å, 2.68 Å, 2.45 Å, 2.06 Å, 1.79 Å, and 1.73 Å matching the (221), (122), (212), (240), (401) and (041) reflections of δNi_2Si. It is well documented for Ni contacts on SiC that the SiC dissociates due to the strong reactivity of nickel above 400 °C, and that at ~900 °C the Ni_2Si stable phase is formed leading to carbon accumulation both at the interface and in the metal layer [2, 4, 5]. Additionally, the 850 °C isothermal section of the Ni-SiC-C ternary phase diagram is characterized by the absence of Ni-C compounds and therefore determined by the nickel-silicide, δNi_2Si (orthorhombic phase), which is in equilibrium with both, C and SiC

[7]. In this ternary phase diagram no Ni-SiC tie line exists, therefore, Ni is not in thermodynamic equilibrium with SiC. Thus, the AES profile data, GAXRD results, and the high temperature Ni-SiC phase equilibria, strongly support the existence of the Ni-Si reaction product, Ni_2Si, spatially adjacent to the SiC substrate. The AES depth profile for the 1000 °C annealed composite contact indicates that both the WSi and the Ti layers served to confine the residual carbon which was released from the dissociation of the SiC during the annealing process. These reactions, W-C and Ti-C, are extremely desirable from the standpoint of device reliability. Carbon inclusions at the metal-SiC interface and within the Ni_2Si contact layer are considered a potential source of electrical instability, especially after prolonged operation of the devices at high temperatures. At elevated temperatures redistribution of carbon inclusions will arise, resulting in significant degradation of the contact's electrical and microstructural properties. Thus, the WSi and Ti layers served to mitigate carbon segregation at the metal-SiC interface.

Carbon inclusions/segregation, are not the only reason for high power and temperature device operation reliability problems. The microstructure of the contact-SiC interface and nature of the contact surface both strongly influence device operational reliability. It has been established that annealing of Ni contacts on SiC causes extensive voiding (Kirkendall voids) at the original metal-SiC interface, a contact thickness which has been substantially expanded, and extreme surface roughness [5, 8]. The voids at the interface will cause internal stress and possible delamination of the contact layer which will compromise device reliability. The internal stress and contact delamination will be significantly amplified under the extreme thermal and electrical stresses typical of the power device operational environment and will ultimately result in device failure. For device applications, ohmic contacts must be wire bonded to a die package. A rough surface morphology will most likely cause wire bonding difficulty and/or failure under the extreme thermal fatigue during high power and high temperature device operation.

Figure 3 displays the FESEM secondary electron cross-sectional images of the as-deposited and 1000 °C annealed contacts to SiC. The metal-SiC interfaces are morphologically abrupt and show no evidence of void formation or contact delamination as a result of the annealing process up to 1000 °C. The distinct metal layers in the as-deposited contact are noted in Fig. 3a. Comparison of the as-deposited and 1000 °C annealed FESEM images in Fig. 3 not only confirms the abrupt void free interface morphology but also reveals that there is minimal increase (<6%) in contact thickness as a result of annealing. Suppression of contact expansion during annealing is due to restricted interfacial contact growth, that is, a narrow Ni-SiC reaction zone. Specifically, deposition of a thin Ni layer, 40 nm, as opposed to the usual 100-200 nm of Ni traditionally employed results in a significantly limited Ni-SiC reaction zone. This mitigated contact growth after heat treatment makes the Pt/Ti/WSi/Ni composite contact an excellent choice for device designs, which possess shallow p-n junctions.

Plan-view FESEM analyses determined that the annealed surfaces remain smooth with evidence of grain growth. Quantitative analysis of surface roughness, an AFM plot of the

average surface roughness (R_{av}) as a function of annealing temperature, is displayed in Fig. 4. The extreme smoothness of the as-deposited contact surface is substantiated by a surface roughness value, R_{av}, of ~0.7 nm. This value remains essentially constant throughout all the heat treatments. Thus, the surface morphology of the annealed composite contact possesses the smoothness required for strong reliable wire bonding and should maintain excellent wire-contact mechanical durability during high power/temperature device operation.
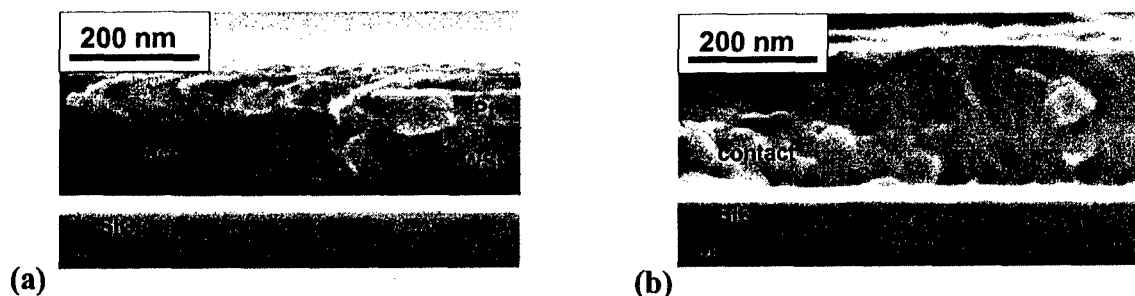

Figure 3: Cross-sectional FESEM micrographs of the (a) as-deposited and (b) 1000 °C annealed Pt/Ti/WSi/Ni composite contact to n-SiC.
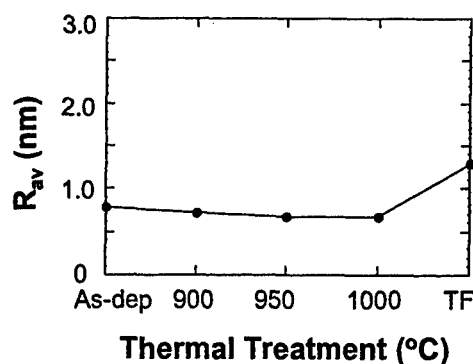

Figure 4: AFM data showing the average surface roughness, R_{av}, of the Pt/Ti/WSi/Ni contact to n-SiC as a function of annealing temperatures up to 1000 °C. TF represents the R_{av} of the 1000 °C annealed contact after exposure to 100 cycles of thermal fatigue at 650 °C.

In order to evaluate device component performance-reliability for pulsed power and /or high power device applications the anneal-optimized (RTA at 950 and 1000 °C for 30 s) Pt/Ti/WSi/Ni-SiC ohmic contacts were subjected to pulsed thermal fatigue testing for up to 100 cycles at 650 °C. The current-voltage characteristics were assessed after exposure to 1, 10 and 100 cycles of thermal fatigue and are displayed in Fig. 5. Figure 5 shows that the contacts initially annealed at both temperatures exhibited similar electrical performance in response to the pulsed thermal stress. The I-V characteristics remained stable, showing little deviation from that of the initial annealed ohmic contact, after exposure to 100 cycles of pulsed thermal fatigue at 650 °C. Assessment of the microstructure in response to pulsed thermal fatigue was achieved via cross-sectional FESEM. The microstructure of the ohmic

contact exposed to 100 cycles of thermal fatigue at 650 °C appeared similar in structure to that of the un-fatigued contact. The fatigued contact exhibited no evidence of nanocracks, or other structural defects associated with potential physical-mechanical contact failure. The fact that the electrical integrity and metal-SiC interfacial microstructure were not significantly altered by the pulsed thermal cycling bodes well for the use of this ohmic contact in pulsed high power devices.
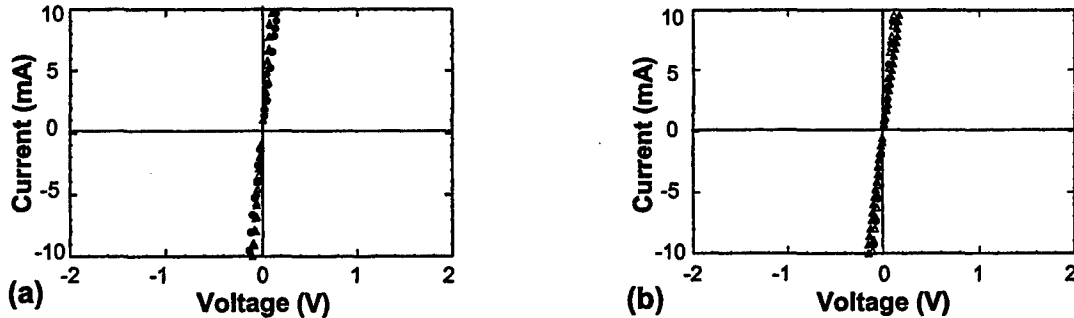

(a)

(b)

Figure 5: I-V characteristics of the 650 °C pulsed thermal fatigued contact initially annealed at (a) 950 °C and (b) 1000 °C. The initial annealed contacts are represented by filled circles and the samples fatigued for 10 and 100 cycles are represented by open and filled triangles, respectively.

For device applications, ohmic contacts must be wire bonded to a die package. Maintenance of a smooth surface morphology is essential to insure good wire bonding and uniformity of current flow. A post fabrication anneal or fatigue-induced rough surface morphology (tens to hundreds of nanometers) will most likely cause wire bond failure. Temperature-induced surface roughness, indicative of interface roughness, which generates excessive stress in the underlying SiC substrate, can result in a SiC polytype change, which causes modification of the device's electrical properties. Quantitative analysis of surface roughness, via AFM, for both the un-fatigued and pulsed thermal fatigued contacts is shown in Fig. 4. The contacts annealed at both annealing temperatures exhibited extremely smooth surfaces. However, after 100 cycles of pulsed thermal fatigue the contacts surface morphology exhibited an increase in the average surface roughness, from 0.7 nm (initial annealed contact) to 1.3 nm. This increase in surface roughness is minimal with respect to the contact thickness, and the actual value of R_{av} is substantially less that other that of other un-fatigued annealed ohmic contacts cited in the technical literature [3, 5]. Thus, the average surface roughness, before and after exposure to pulsed thermal fatigue, is considered negligible and should not be an influencing factor for wire bond failure and/or electrical degradation. Additionally, the fact that the contact metal did not delaminate as a result of the thermal cycling indicates strong adhesion of the metal contact to the SiC substrate.

Static thermal fatigue/aging experiments were performed on the contacts in order to evaluate their performance for high temperature device applications. Identical contacts to those utilized for pulsed thermal fatigue testing, (initially annealed at both 950 and 1000 °C)

were exposed to static thermal stability/aging tests for various times up to 100 h at 650 °C in an N_2 ambience. The contacts were electrically evaluated after 1, 24, 50, 75, and 100 hrs of aging, and the I-V characteristics of the initially annealed (950 and 1000 °C) and static thermally fatigued contacts are shown in Fig. 6. The I-V characteristics of the 950 °C annealed ohmic contacts aged for up to 50 h maintained good ohmicity, however, an increase in resistance with respect to that of the un-aged contact was noted. This contact became rectifying after 75 h of aging. In contrast, the 1000 °C annealed ohmic contact maintained I-V linearity, with an increase in resistance, after aging for up to 75 h. After 100 h of aging the I-V characteristics exhibited a further increase in resistance, however, the contact did not become rectifying. Thus, the ohmic contact which had been initially annealed at 1000 °C, appears to be more electrically stable in response to long term aging than the 950 °C annealed ohmic contact.
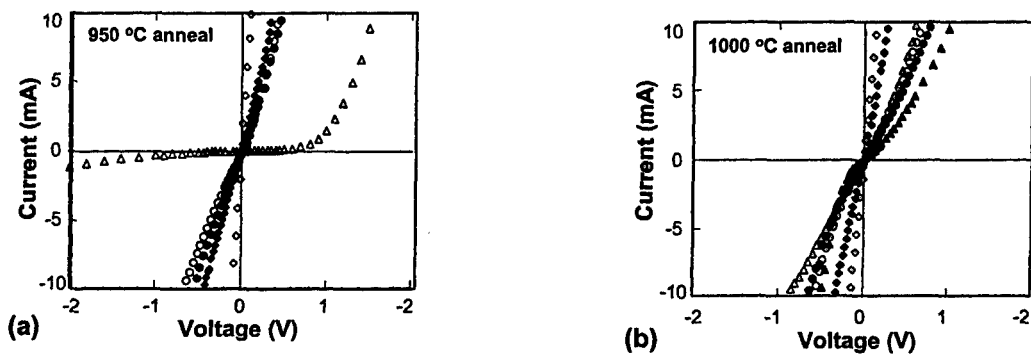

Figure 6: I-V characteristics of the 650 °C aged Pt/Ti/WSi/Ni-nSiC ohmic contacts initially annealed at (a) 950 °C for 30 s and (b) 1000 °C for 30 s. The initial annealed samples are represented by open diamonds, and the samples aged for 1, 24, 50, 75 and 100 h are represented by filled diamonds, open circles, filled circles, open triangles, and filled triangles, respectively.

In order to identify the source(s) of degradation of the aged 950 °C annealed ohmic contact, the 950 and 1000 °C annealed contacts were characterized via FESEM and RBS. The cross-sectional microstructure of the 950 and 1000 °C annealed contacts after exposure to 75 h of aging appeared identical. The metal-SiC interface appeared structurally abrupt with no evidence of degradation via metal-SiC interface modification. The surface morphology of both samples also appeared similar, with no evidence of thermally induced surface heterogeneity, roughening, nanocracks or pit formation. The RBS spectra for the annealed contacts (RTA at 950 and 1000 °C for 30 s) before and after aging (650 °C for 75 h) are displayed in Fig. 7. The static thermal fatigue/aging treatment of the 950 °C contact modified the RBS spectrum, with respect to that of the unaged 950 °C annealed contact, by shifting the "back edge" of the RBS peak (around 1440 keV) to a lower energy (Fig. 7a). This shift is indicative of a net movement of the contact material into the SiC substrate in response to the long-term static thermal fatigue/aging. Figure 7b shows that the back edge of

the 1000 °C contact metallization remained relatively unchanged after the same treatment, indicating that the contact-SiC interface experienced little or no reaction/diffusion. This result is in agreement with the electrical measurements which showed rectifying characteristics for the 75 h aged 950 °C annealed contact and ohmic behavior for the 1000 °C annealed contact aged for 100 h. The RBS results suggest that the 1000 °C annealed Pt/Ti/WSi/Ni contact must have undergone a more complete interfacial reaction with the SiC during the initial annealing process such that the driving force for any further interfacial reaction was exhausted. In contrast, the fact that the 950 °C annealed contact experienced elemental diffusion and/or interfacial reactions which resulted in electrical degradation after long term aging suggests that the metal-SiC had not fully reacted at the initial annealing temperature of 950 °C. Thus, even though this contact initially displayed acceptable electrical behavior after annealing at 950 °C, exposure to prolonged thermal aging at 650 °C caused the electrical integrity of the contact to degrade. The results suggest that the 950 °C annealed contact was not in complete thermodynamic equilibrium with SiC, and prolonged exposure at elevated temperature during aging allowed the contact metallization to continue to react with the SiC substrate, resulting in electrical degradation.
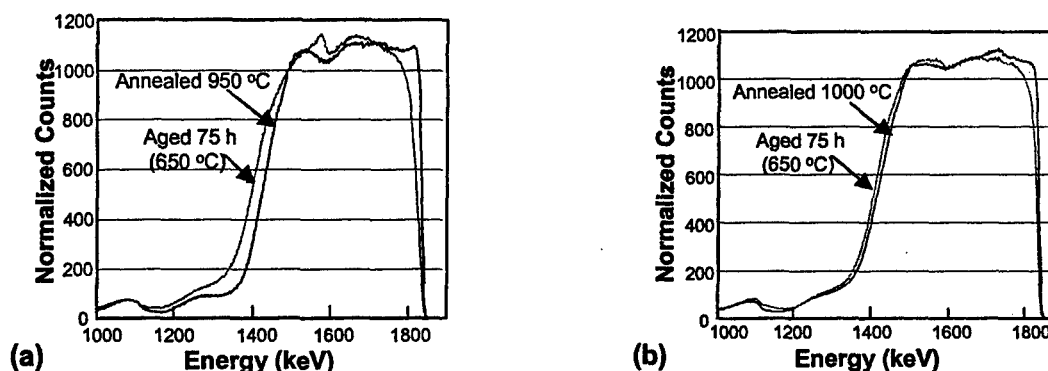

Figure 7: RBS spectra of the Pt/Ti/WSi/Ni ohmic contacts to n-SiC aged for 75 h at 650 °C subsequent to the initial anneals at (a) 950 °C and (b) 1000 °C for 30 s.

IV. SUMMARY

We have achieved excellent electrical properties for Pt/Ti/WSi/Ni ohmic contacts to n-SiC annealed between 950 and 1000 °C for 30 s. The excellent electrical properties were paralleled by the formation of a narrow Ni_2Si interfacial reaction zone, minimal contact broadening, and a smooth, abrupt, and void free contact-SiC interface. The residual carbon, resultant from the reaction of SiC with the overlying Ni, was confined by Ti-carbide and W-carbide phases spatially distant from the contact-SiC interface. Thus, the detrimental effects of contact delamination due to stress associated with interfacial voiding, and wire bond failure due to extreme surface roughness, have been eliminated for this composite ohmic contact. Additionally, electrical instability associated with carbon inclusions at the contact-SiC interface after prolonged high temperature and high power device operation has also

been eliminated. The thermal stability of Pt/Ti/WSi/Ni ohmic contacts to n-SiC was assessed via acute pulsed/cyclic thermal fatigue and long term thermal aging experiments. The 950 and 1000 °C annealed ohmic contacts exhibited excellent electrical and microstructural stability in response to acute pulsed thermal fatigue at 650 °C for up to 100 cycles. The absence of observed surface and metal-SiC interfacial modification in combination with the stable electrical characteristics demonstrates strong potential for application of this contact metallization in pulsed power device applications. Aging at 650 °C resulted in contact failure for the 950 °C annealed contact after 75 hours and ohmic behavior for the 1000 °C annealed contact after 100 hours of exposure. The RBS results indicate that the 1000 °C annealed contact underwent complete interfacial reaction with SiC during the initial anneal, but the 950 °C annealed contact experienced further elemental diffusion and/or interfacial reactions in response to prolonged exposure at elevated temperature, resulting in electrical degradation. It is suggested that oxidation of both contacts contributed to the slight increase in contact resistance observed during aging. Results of this investigation demonstrates that the 1000 °C annealed Pt/Ti/WSi/Ni ohmic contact to n-SiC merits beneficial potential for both high temperature and high (pulsed) power device applications.

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